

chain nodes :

6 11 12 13 14 17 19 20 21

ring nodes :

1 2 3 4 5 7 8 9 10

chain bonds :

4-6 5-20 7-11 8-17 9-12 10-19 13-14 20-21

ring bonds :

1-2 1-5 2-7 3-4 3-10 4-5 7-8 8-9 9-10

exact/norm bonds :

4-6 5-20 7-11 8-17 9-12 10-19

exact bonds :

1-2 1-5 2-7 3-4 3-10 4-5 7-8 8-9 9-10 13-14 20-21

isolated ring systems :

containing 1 :

G1:CH2, [*1]

G2:CH3, Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 17:CLASS 19:CLASS 20:CLASS 21:CLASS

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NEWS	9	Oct 27	New Extraction Code PAX now available in Derwent Files
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=> file reg

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SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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0.15

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DICTIONARY FILE UPDATES: 1 NOV 2000 HIGHEST RN 300762-14-5

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when
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Structure search limits have been increased. See HELP SLIMIT
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=>

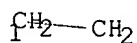
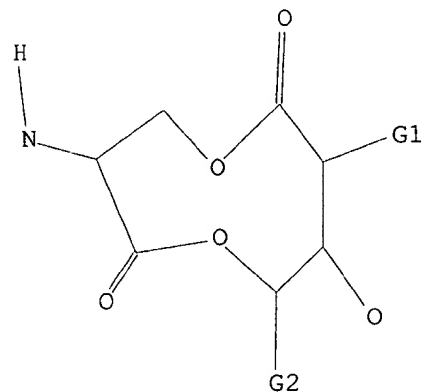
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 CH2, [01]

G2 Me, Et

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 12:40:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS
SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 561 TO 1399
PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=>

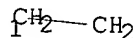
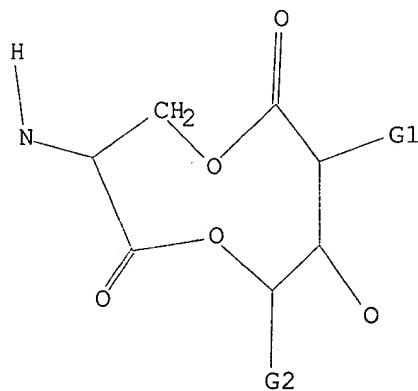
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L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



G1 CH2, [01]

G2 Me, Et

Structure attributes must be viewed using STN Express query preparation.

=> s 13

SAMPLE SEARCH INITIATED 12:41:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 561 TO 1399
PROJECTED ANSWERS: 4 TO 200

L4 4 SEA SSS SAM L3

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 126.00 U.S. DOLLARS
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FULL SEARCH INITIATED 12:41:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1140 TO ITERATE

100.0% PROCESSED 1140 ITERATIONS 75 ANSWERS
SEARCH TIME: 00.00.05

L5 75 SEA SSS FUL L3

=> file ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	127.20	127.35

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FILE LAST UPDATED: 27 Oct 2000 (20001027/ED)

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=> s 15

L6 14 L5

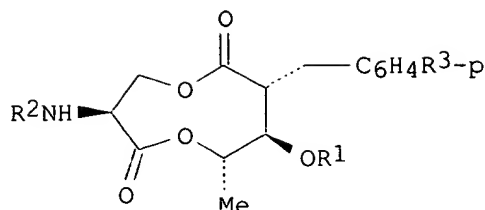
=> s 16 and sakanaka, o?/au

21 SAKANAKA, O?/AU
L7 3 L6 AND SAKANAKA, O?/AU

=> d 17, ibib abs fhitr, 1-3

L7 ANSWER 1 OF 3 CA COPYRIGHT 2000 ACS
ACCESSION NUMBER: 131:129825 CA
TITLE: Novel antifungal compounds and process for producing the same
INVENTOR(S): **Sakanaka, Osamu**; Teraoka, Takeshi; Mitomo, Koichi; Tamura, Takayoshi; Murai, Yasushi; Iinuma, Katsuharu; Kuzuhara, Kikuko; Mikoshiba, Haruki; Taniguchi, Makoto
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9940081	A1	19990812	WO 1999-JP541	19990208
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9924398	A1	19990823	AU 1999-24398	19990208
PRIORITY APPLN. INFO.:			JP 1998-26257	19980206
			WO 1999-JP541	19990208
OTHER SOURCE(S):		MARPAT 131:129825		
GI				



I

AB The title compds. [I; R1 = iso-Bu, tigloyl, isovaleryl, 2-methylbutanoyl; R2 = H, arom. acyl, protecting group such substituted benzoyl, substituted

nicotinoyl; R3 = H, nitro, amino, acylamino, N,N-dialkylamino; with provisos] are prepd. Thus, UK-2A in CH₂Cl₂ contg. pyridine and PCl₅ was refluxed for 1.5 h, the reaction mixt. was allowed to cool and then reacted with methanol for 15 h to give

(2R,3R,4S,7S)-7-amino-2-benzyl-5,9-dioxo-3-isobutyryloxy-4-methyl-1,6-cyclononanedione. In an antifungal test, (2R,3R,4S,7S)-7-(2-hydroxynicotinylamino)-2-benzyl-5,9-dioxo-3-isobutyryl-4-methyl-1,6-cyclononanedione (also prepd.) at 0.05 .mu.g showed potency almost double that of UK-2A against *Saccharomyces cerevisiae*.

IT **234112-85-7P**

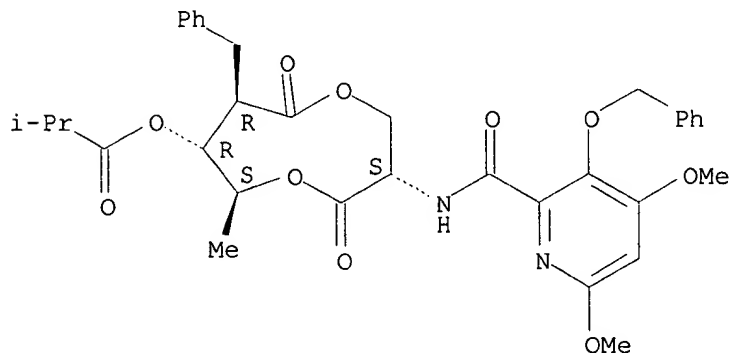
RL: BAC (Biological activity or effector, except adverse); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of UK-2A derivs. as antifungals)

RN 234112-85-7 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4,6-dimethoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

4

REFERENCE(S):

(1) Kobe Steel Ltd; JP 07-196489 A 1969

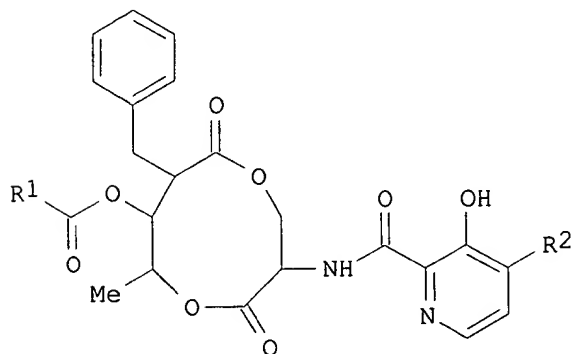
(2) Kyowa Fermentation Industry Co, Ltd; JP 44-235 B

1969

(3) Shimano, M; Tetrahedron 1998, V54(42), P12745 CA
 (4) Suntory Ltd; JP 07-233165 A 1995

L7 ANSWER 2 OF 3 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 130:193104 CA
 TITLE: Rice blast controlling agents and wheat scab
 controlling agents
 INVENTOR(S): Teraoka, Takeshi; Kuzuhara, Kikuko; Mikoshiba,
 Haruki;
 Matsumoto, Kuniomi; Iinuma, Katsuharu; Futamura,
 Takafumi; Yasutake, Tetsuya; **Sakanaka, Osamu**
 ; Mitomo, Koichi; Taniguchi, Makoto
 PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
 SOURCE: PCT Int. Appl., 24 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911127	A1	19990311	WO 1998-JP3876	19980831
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9888878	A1	19990322	AU 1998-88878	19980831
EP 1013169	A1	20000628	EP 1998-940634	19980831
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
PRIORITY APPLN. INFO.:			JP 1997-233658	19970829
			WO 1998-JP3876	19980831
OTHER SOURCE(S):	MARPAT 130:193104			
GI				

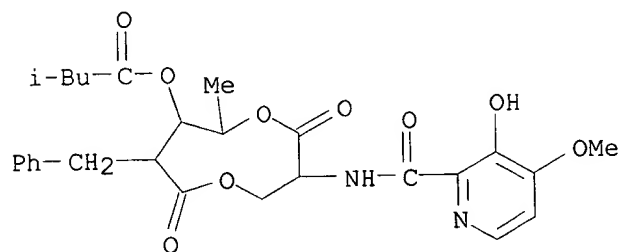


I

AB These agents contain a compd. represented by formula (I) in which R1 represents alkyl or alkenyl and R2 represents hydrogen or methoxy. The compd. is highly effective in preventing rice blast and wheat scab and is not injurious to the plants. Specific compds. used in the examples are obtained by the method described in a publication presented earlier. Activities of I where R1 = iso-Pr and R2 = H (1), R1 = iso-Pr and R2 = OMe (2), R1 = (Z)-2-butenyl and R2 = OMe (3), R1 = iso-Bu and R2 = OMe (4), and R1 = sec-Bu and R2 = OMe (5), were demonstrated.

IT **167173-87-7**
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BIOL (Biological study); USES (Uses)
 (as rice blast controlling agents and wheat scab controlling agents)

RN 167173-87-7 CA
 CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

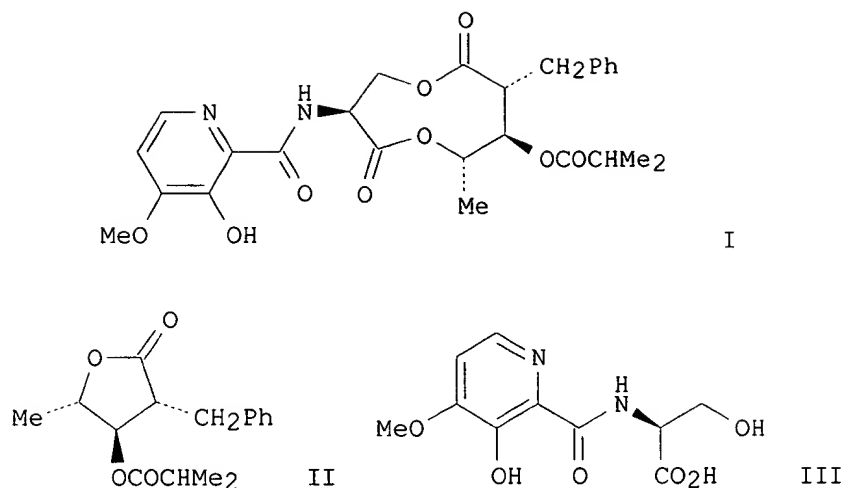


REFERENCE COUNT: 3
 REFERENCE(S): (1) Hanafi; Journal of Antibiotics 1996, V49(12), P1226 CA
 (2) Suntory Ltd; JP 07-233165 A 1995
 (3) Ueki; Journal of Antibiotics 1997, V50(7), P551

CA

L7 ANSWER 3 OF 3 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 130:168617 CA
 TITLE: UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 III. Absolute configuration of an antifungal antibiotic, UK-2A, and consideration of its conformation
 AUTHOR(S): Shibata, Kozo; Hanafi, Muhammad; Fujii, Jyunko; Sakanaka, Osamu; Iinuma, Katsuharu; Ueki, Masashi; Taniguchi, Makoto
 CORPORATE SOURCE: Faculty of Science, Osaka City University, Osaka, 558-8585, Japan
 SOURCE: J. Antibiot. (1998), 51(12), 1113-1116
 CODEN: JANTAJ; ISSN: 0021-8820
 PUBLISHER: Japan Antibiotics Research Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English

GI



AB The abs. configuration of UK-2A (I) was detd. by the elucidation of the abs. configurations of butanolide II and the serine deriv. III, the products of alk. hydrolysis of I. The abs. configuration of UK-2A was found to be (+)-(2R,3R,4S,7S).

IT 167173-86-6, UK 2B

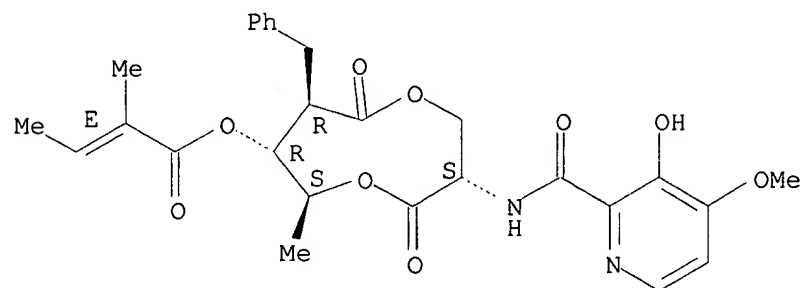
RL: MSC (Miscellaneous)

(detn. of the abs. configuration of UK-2A, an antifungal antibiotic)

RN 167173-86-6 CA

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT:
REFERENCE(S):

6

- (1) Fujii, K; Synthesis 1975, P276 CA
- (2) Hanafi, M; J Antibiotics 1996, V49, P1226 CA
- (3) Trecourt, F; Tetrahedron 1993, V49, P8373 CA
- (4) Ueki, M; J Antibiotics 1996, V49, P639 CA

(5) Wasserman, H; Chem Rev 1986, V86, P845 CA
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 12:39:26 ON 02 NOV 2000)

FILE 'REGISTRY' ENTERED AT 12:39:46 ON 02 NOV 2000

L1 STRUCTURE UPLOADED
L2 7 S L1
L3 STRUCTURE UPLOADED
L4 4 S L3
L5 75 S L4 FULL

FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000

L6 14 S L5
L7 3 S L6 AND SAKANAKA, O?/AU

=> s 16 not 17

L8 11 L6 NOT L7

=> s 18 and pd < march 1998

14800117 PD < MARCH 1998
(PD<19980300)

L9 9 L8 AND PD < MARCH 1998

=> d 19, ibib abs hitstr, 1-9

L9 ANSWER 1 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER: 131:214101 CA

TITLE: Total synthesis of the antifungal dilactone UK-2A and
 analogs and their bioactivities

AUTHOR(S): Kamei, Noriyuki; Shibata, Tetsuo; Inoguchi, Kiyoshi;
 Senda, Hisato; Ikari, Takashi; Itoh, Nobuko; Shimano,
 Masanao

CORPORATE SOURCE: Department of Medical Chemistry and Molecular Design,
 Drug Discovery Research Laboratories, Kaken
 Pharmaceutical Co., Ltd., Japan

SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (
 1998), 40th, 679-684

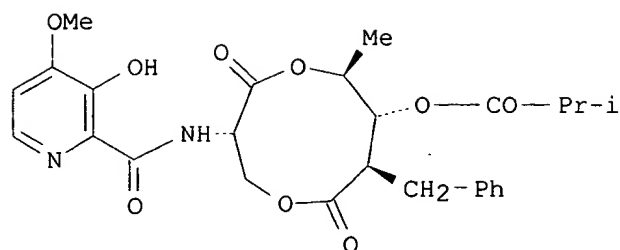
CODEN: TYKYDS

PUBLISHER: Nippon Kagakkai

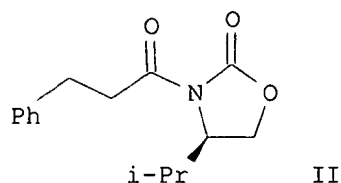
DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



103

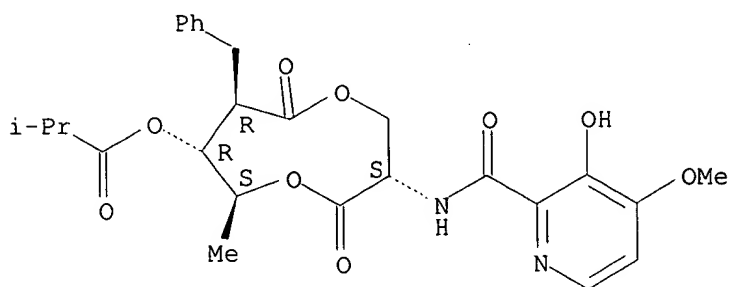


AB UK-2A (I) which has recently been isolated from the mycelial cake of *Streptomyces* sp. 517-02, possesses nine-membered dilactone and a picolinic acid moiety. The plane structure of UK-2A has been elucidated by ¹H and ¹³C NMR analyses and chem. degrdn. studies, but the relative and abs. configurations of the four chiral centers in UK-2A still remain to be detd. UK-2A has strongly inhibited the growth of various kinds of yeasts and filamentous fungi, but its cytotoxic activities against several kinds of mammalian cells were very weak. The combination of its interesting mol. architecture and the potent antifungal activity prompted us to launch the total synthesis of UK-2A. The synthesis of UK-2A has been achieved through a 12-step sequence from II in 26% overall yield. The key strategy employed in this approach involves; (1) construction of the three consecutive chiral centers from C2 to C4 based upon the well-established Evans aldol reaction and (2) the nine-membered lactonization. The authors' synthetic route to UK-2A would permit a practical and reliable construction of UK-2A and a variety of its analogs. In order to define the selective cytotoxicities of UK-2A against yeasts and filamentous fungi, UK-2A and its analogs synthesized were subjected to the MIC evaluation and cytotoxic activity examn. compared with the ref. compds., amphotericin B and fluconazole. UK-2A has a broad antifungal spectrum, while its cytotoxicities was considerably weak compared to other substrates. The results of the UK-2A analogs suggested that the basicity of the picolinic acid moiety in UK-2A was essential for the antifungal activities and that the feature of the nine-membered dilactone contributed to the selective cytotoxicities.

IT **167173-85-5P**, Antibiotic UK 2A
 RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (total synthesis of antifungal dilactone UK-2A and analogs and bioactivities)

RN 167173-85-5 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

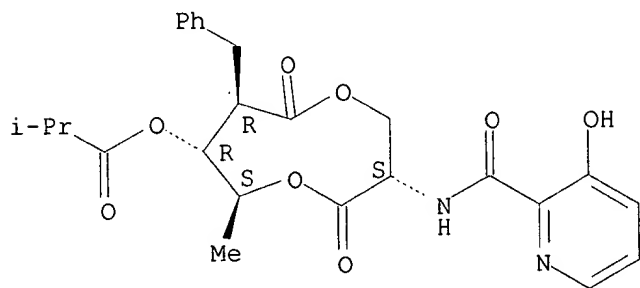


IT 194931-82-3P 210426-79-2P 215798-04-2P
 215798-05-3P 215798-17-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (total synthesis of antifungal dilactone UK-2A and analogs and bioactivities)

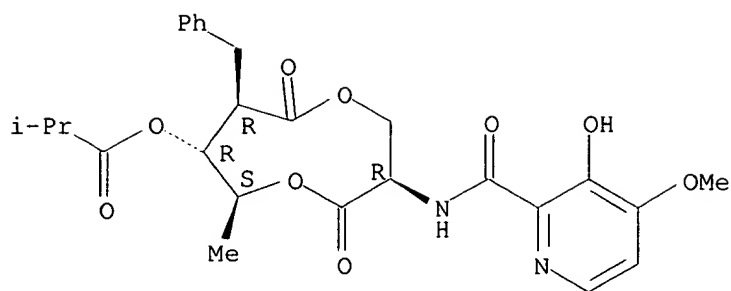
RN 194931-82-3 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 210426-79-2 CA
 CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

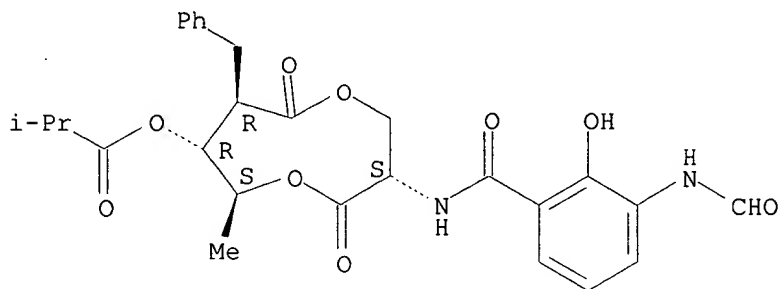
Absolute stereochemistry. Rotation (+).



RN 215798-04-2 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

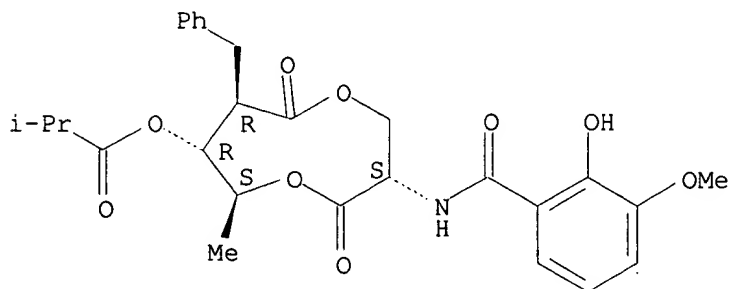
Absolute stereochemistry. Rotation (+).



RN 215798-05-3 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

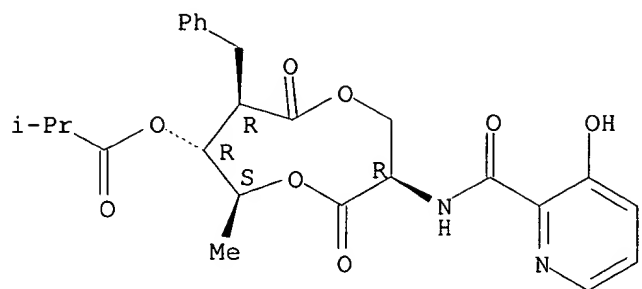
Absolute stereochemistry. Rotation (+).



RN 215798-17-7 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[[3-hydroxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



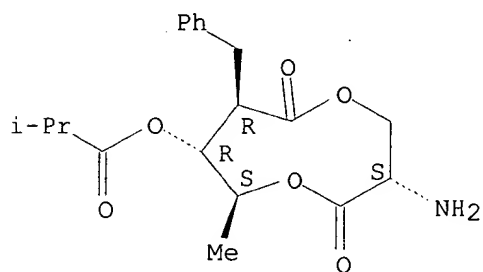
IT 210300-07-5P 210300-13-3P 210300-18-8P
215798-00-8P 215798-10-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of antifungal dilactone UK-2A and analogs and
bioactivities)

RN 210300-07-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

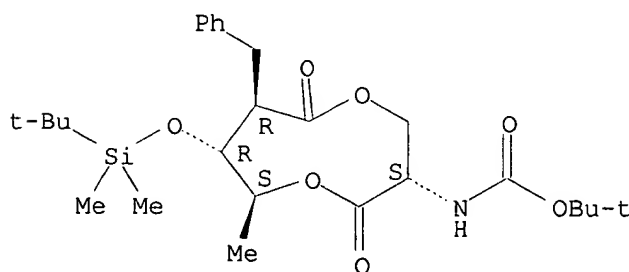
Absolute stereochemistry.



RN 210300-13-3 CA

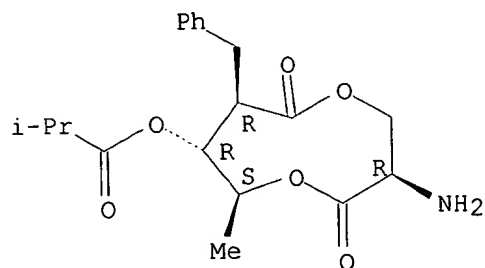
CN Carbamic acid,
[(3S,7R,8R,9S)-8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



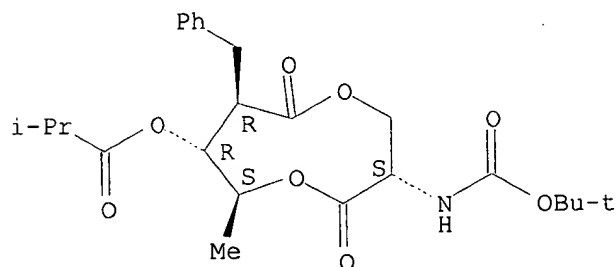
RN 210300-18-8 CA
 CN Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



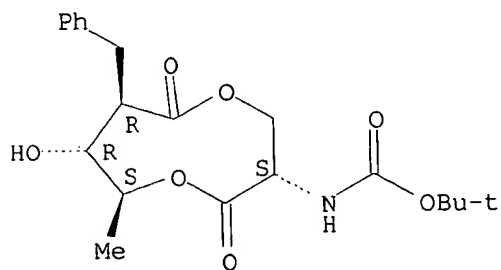
RN 215798-00-8 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

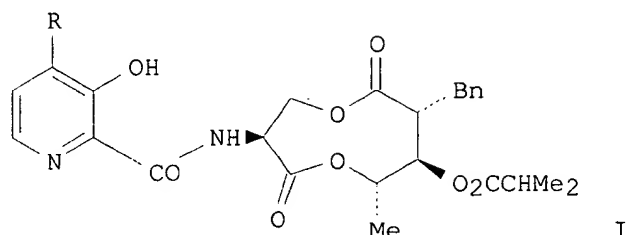


RN 215798-10-0 CA
 CN Carbamic acid, [(3S,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 2 OF 9 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 130:3703 CA
 TITLE: Total synthesis of the antifungal dilactones UK-2A
 and UK-3A: the determination of their relative and
 absolute configurations, analog synthesis and
 antifungal activities
 AUTHOR(S): Shimano, Masanao; Kamei, Noriyuki; Shibata, Tetsuo;
 Inoguchi, Kiyoshi; Itoh, Nobuko; Ikari, Takashi;
 Senda, Hisato
 CORPORATE SOURCE: Dep. Med. Chem. Mol. Design, Drug Discovery Res.
 Lab., Kaken Pharmaceutical Co., Ltd., Minami Kawara-cho,
 Yamashina-ku, Kyoto, 607-8042, Japan
 SOURCE: Tetrahedron (1998), 54(42), 12745-12774
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 130:3703
 GI



AB The synthesis of the antifungal dilactones (I), UK-2A (R = OMe) and UK-3A (R = H), is described. In addn. to providing a workable synthetic route to these potent antifungal antibiotics, this has allowed us to det. the assignment of the relative and abs. configurations in the nine-membered ring. Furthermore, UK-2A analogs were also synthesized and evaluated for their antifungal activities and cytotoxic activities along with UK-2A, (2R, 3R, 4S, 7R)-UK-2A, UK-3A, (2R, 3R, 4S, 7R)-UK-3A, and antimycin A. The structural requirements for the selective cytotoxicity against yeasts and filamentous fungi will also be suggested.

IT 167173-85-5P, UK-2A 194931-82-3P, UK-3A
 210426-79-2P 215798-04-2P 215798-05-3P
 215798-17-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis, antifungal activity, cytotoxicity and abs. configuration

of

dilactones UK-2A and UK-3A)

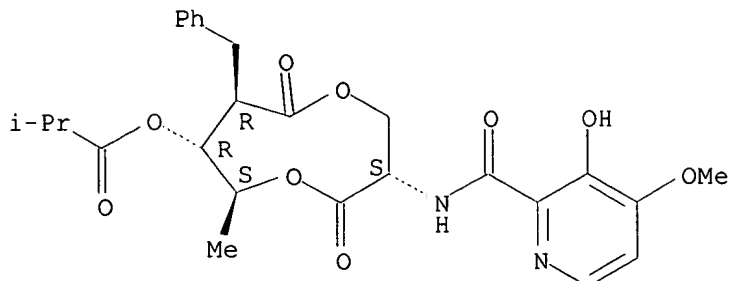
RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl) carbonyl] amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxo-
 Page 16

7-yl ester (9CI) (CA INDEX NAME)

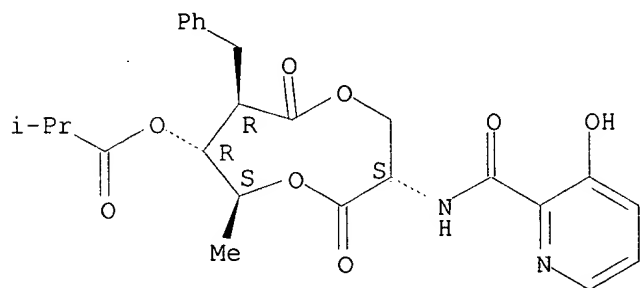
Absolute stereochemistry. Rotation (+).



RN 194931-82-3 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-hydroxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

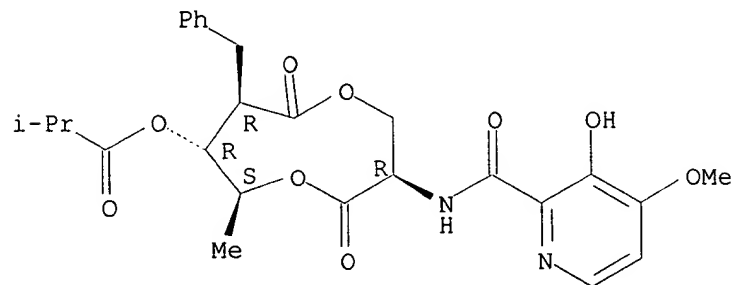


103

RN 210426-79-2 CA

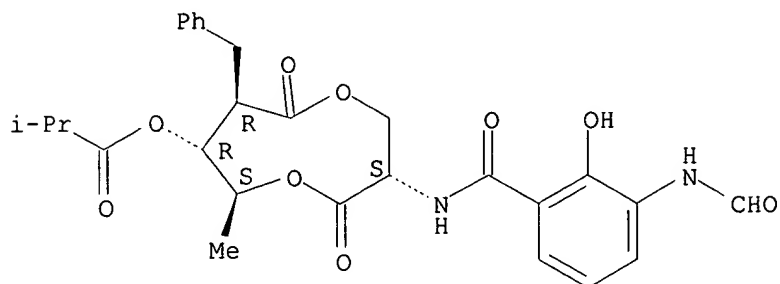
CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[[3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



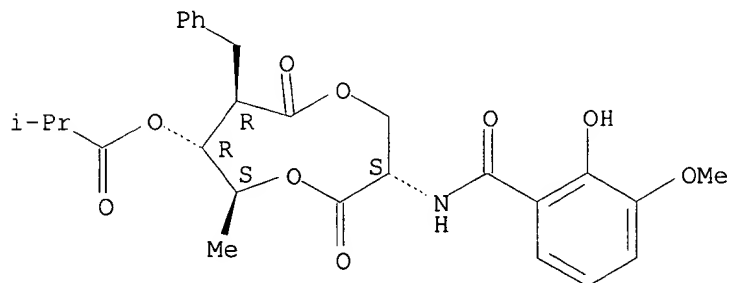
RN 215798-04-2 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



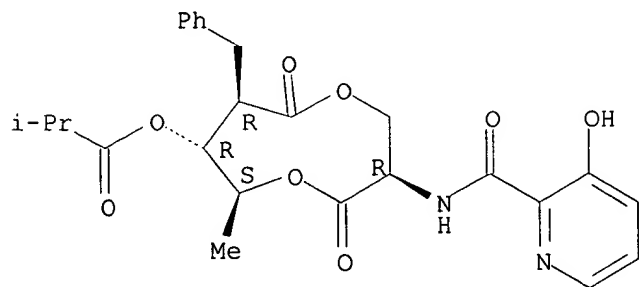
RN 215798-05-3 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

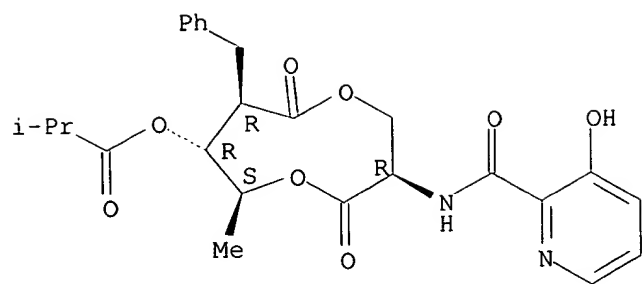
Absolute stereochemistry. Rotation (+).



RN 215798-17-7 CA
 CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[3-(3-hydroxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).





IT 210300-07-5P 210300-13-3P 210300-17-7P
 210300-18-8P 215798-00-8P 215798-10-0P
 215798-15-5P 215798-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis, antifungal activity, cytotoxicity and abs. configuration

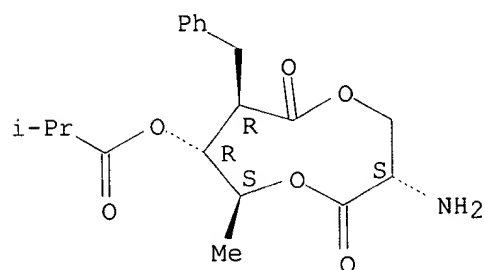
of

dilactones UK-2A and UK-3A)

RN 210300-07-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

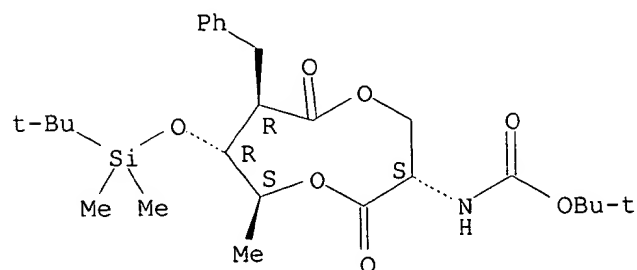


RN 210300-13-3 CA

CN Carbamic acid,

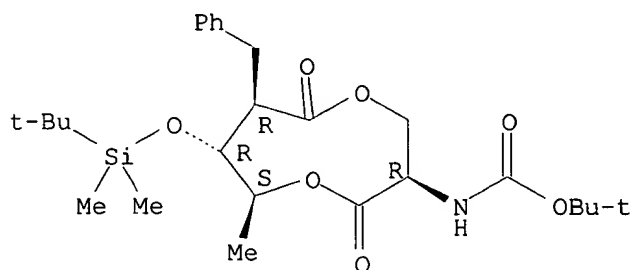
[(3S,7R,8R,9S)-8-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



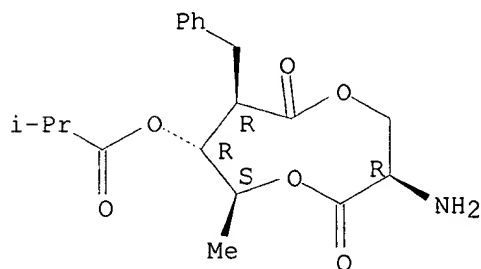
RN 210300-17-7 CA
 CN Carbamic acid,
 [(3R,7R,8R,9S)-8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-
 methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl
 ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



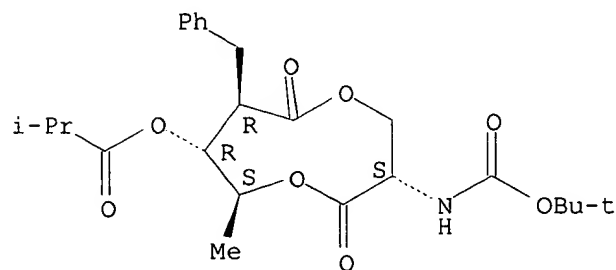
RN 210300-18-8 CA
 CN Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-
 (phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



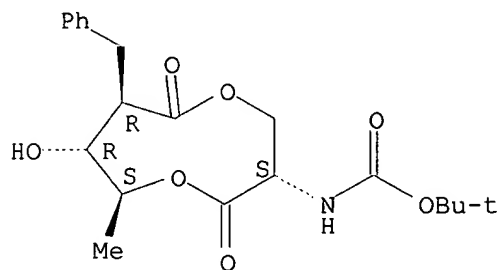
RN 215798-00-8 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(1,1-
 dimethylethoxy)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-
 dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



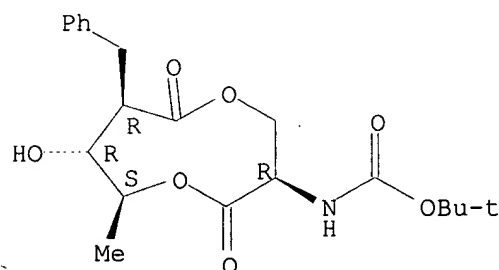
RN 215798-10-0 CA
 CN Carbamic acid, [(3S,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



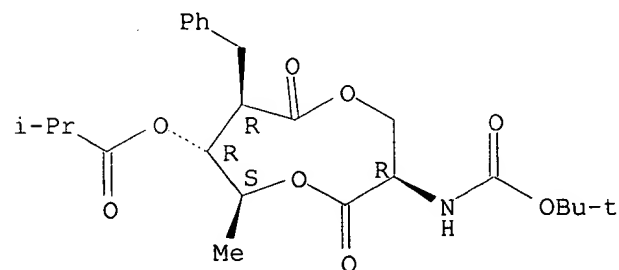
RN 215798-15-5 CA
 CN Carbamic acid, [(3R,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



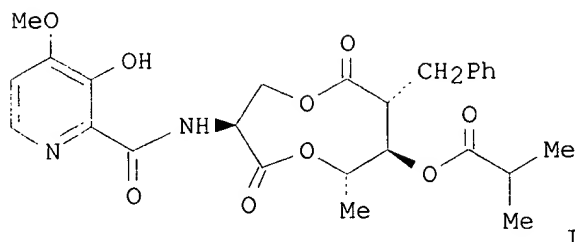
RN 215798-16-6 CA
 CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



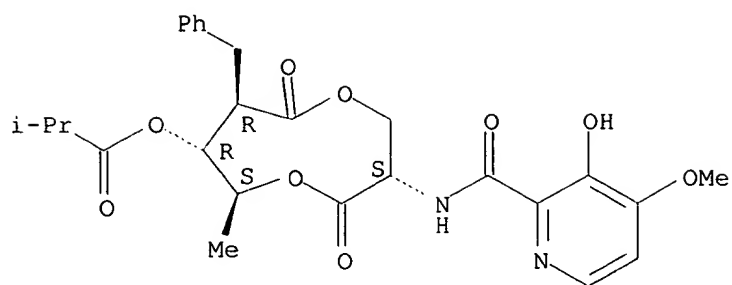
REFERENCE COUNT: 36
 REFERENCE(S): (2) Barrow, C; J Antibiot 1997, V50, P729 CA
 (3) Brooks, B; J Comput Chem 1983, V4, P187 CA
 (4) Centeno, N; Chem Phys Lett 1995, V232, P374 CA
 (6) Evans, D; J Am Chem Soc 1981, V103, P2127 CA
 (7) Evans, D; J Am Chem Soc 1982, V104, P1737 CA
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 9 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 129:122477 CA
 TITLE: Enantioselective total synthesis of the antifungal dilactone, UK-2A: the determination of the relative and absolute configurations
 AUTHOR(S): Shimano, Masanao; Shibata, Tetsuo; Kamei, Noriyuki
 CORPORATE SOURCE: Dep. Medicinal Chem. Molecular Design, Drug Discovery Res. Labs., Kaken Pharmaceutical Co., Kyoto, 607-8042, Japan
 SOURCE: Tetrahedron Lett. (1998), 39(24), 4363-4366
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 129:122477
 GI



AB The synthesis of the antifungal dilactone, UK-2A (I), is described. In addn. to providing a workable synthetic route to this potent antifungal antibiotic, this has allowed us to det. the assignment of the relative and
 abs. configurations in the nine-membered ring.
 IT **167173-85-5P**, (+)-UK-2A **210426-79-2P**, 7-epi-UK-2A
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (abs. configuration of UK-2A via enantioselective total synthesis)
 RN 167173-85-5 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-hydroxy-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

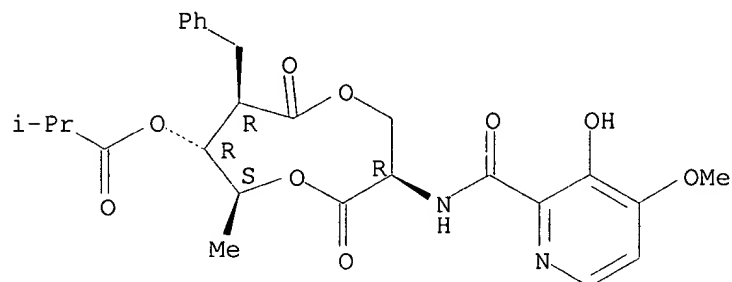
Absolute stereochemistry. Rotation (+).



RN 210426-79-2 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



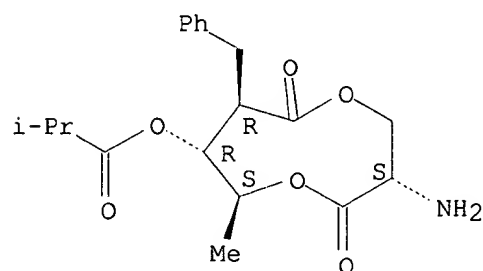
IT 210300-07-5P 210300-13-3P 210300-17-7P
210300-18-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(abs. configuration of UK-2A via enantioselective total synthesis)

RN 210300-07-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

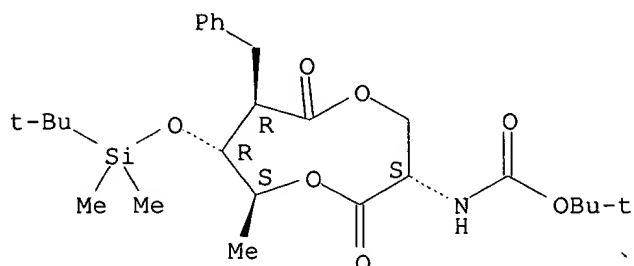


RN 210300-13-3 CA

CN Carbamic acid,
[(3S,7R,8R,9S)-8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-

methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

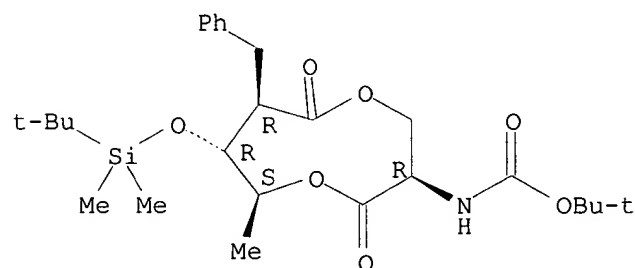


RN 210300-17-7 CA

CN Carbamic acid,

[(3R,7R,8R,9S)-8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

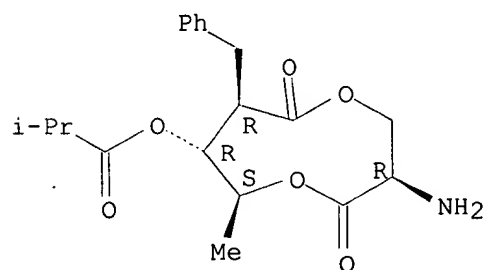
Absolute stereochemistry. Rotation (+).



RN 210300-18-8 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 9 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 128:163891 CA
 TITLE: The mode of action of UK-2A and UK-3A, novel
 antifungal antibiotics from *Streptomyces* sp. 517-02
 AUTHOR(S): Ueki, Masashi; Taniguchi, Makoto
 CORPORATE SOURCE: Dep. Biology, Fac. Sci., Osaka City Univ., Osaka,
 558,
 SOURCE: Japan
 J. Antibiot. (1997), 50(12), 1052-1057
 CODEN: JANTAJ; ISSN: 0021-8820
 PUBLISHER: Japan Antibiotics Research Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB UK-2A and UK-3A are structural relatives of antimycins, which were isolated as antifungal antibiotics with little cytotoxicity that demonstrated inhibition of respiratory activity. They halve the cellular respiration of yeast within 4~5 min and the intracellular ATP content within 2~5 min. They inhibited the yeast mitochondrial respiration using .beta.-hydroxybutyrate and succinate as a respiratory substrate, but no inhibition was obsd. using ascorbate-reduced tetra-Me p-phenylenediamine as the substrate. The site of respiratory inhibition of UK-2A and UK-3A was thought to be the cytochrome bcl complex in the mitochondrial

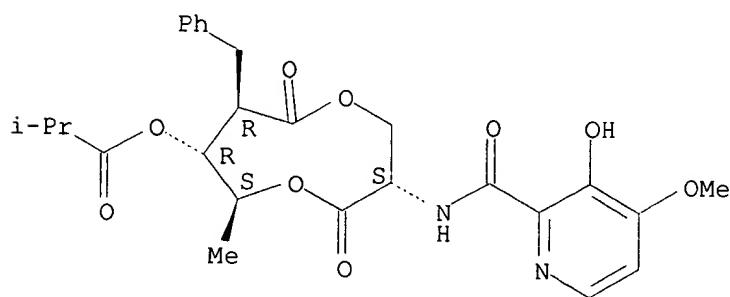
electron transport chain of yeast cells. They also inhibited the mitochondrial respiration of rat liver. Intact animal cells might have some system to defend themselves from the actions of UK-2A and UK-3A.

IT 167173-85-5, UK-2A 194931-82-3, Antibiotic UK-3A
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
 (mechanism of antifungal action of UK-2A and UK-3A)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

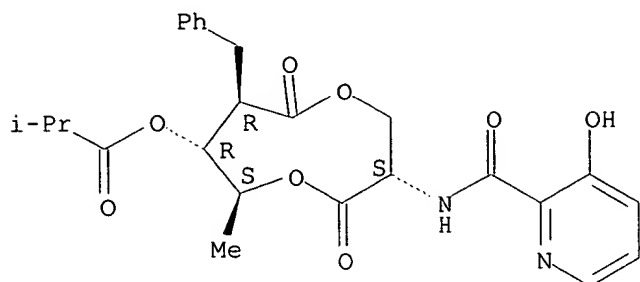
Absolute stereochemistry. Rotation (+).



RN 194931-82-3 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L9 ANSWER 5 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER: 127:217524 CA

TITLE: UK-3A, a novel antifungal antibiotic from
Streptomyces

sp. 517-02: fermentation, isolation, structural
elucidation and biological properties

AUTHOR(S): Ueki, Masashi; Kusumoto, Atsushi; Hanafi, Muhammad;
Shibata, Kozo; Tanaka, Toshio; Taniguchi, Makoto

CORPORATE SOURCE: Faculty of Science, Osaka City University, Osaka,
558,

SOURCE: Japan
J. Antibiot. (1997), 50(7), 551-555

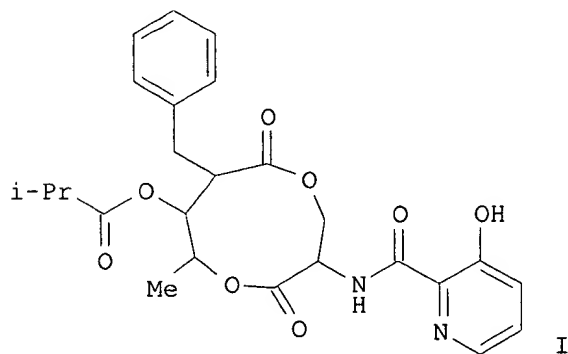
CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



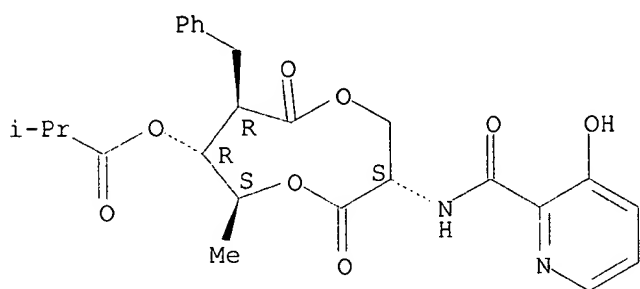
AB A novel antifungal antibiotic, UK-3A (I), was obtained from the mycelial
cake of Streptomyces sp. 517-02. I was very similar in structure to
UK-2A, a structural relative of antimycin A. The antifungal spectrum of

I

was relatively broad (MICs for yeasts and filamentous fungi:
1.56.apprx.6.25 and 0.39.apprx.1.56 .mu.g/mL, resp.). The cytotoxic

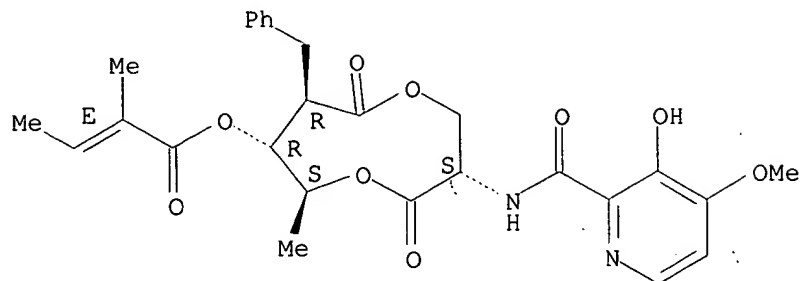
activity of I was weak (IC₅₀: 18.apprx.100 .mu.g/mL).
 IT 194931-82-3P, Antibiotic UK 3A
 RL: BAC (Biological activity or effector, except adverse); BOC
 (Biological occurrence); BPN (Biosynthetic preparation); PRP (Properties); BIOL
 (Biological study); OCCU (Occurrence); PREP (Preparation)
 (UK-3A is a novel antifungal antibiotic from Streptomyces)
 RN 194931-82-3 CA
 CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-
 pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-
 7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

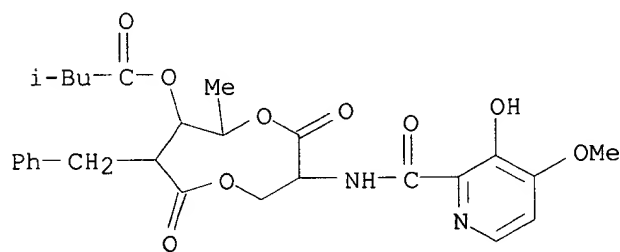


L9 ANSWER 6 OF 9 CA COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 126:144017 CA
 TITLE: UK-2A, B, C and D, novel antifungal antibiotics from
 Streptomyces sp. 517-02. II. Structural elucidation
 AUTHOR(S): Hanafi, Muhammad; Shibata, Kozo; Ueki, Masashi;
 Taniguchi, Makoto
 CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan
 SOURCE: J. Antibiot. (1996), 49(12), 1226-1231
 CODEN: JANTAJ; ISSN: 0021-8820
 PUBLISHER: Japan Antibiotics Research Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB UK-2A, UK-2B, UK-2C and UK-2D, novel antibiotics produced by Streptomyces
 sp. 517-02, exhibit strong antifungal activity. The structures were
 elucidated based on spectral and chem. evidence that these compds. are
 the
 derivs. of the nine-membered dilactone formed from serine and
 4-hydroxypentanoic acid moiety.
 IT 167173-86-6P 167173-87-7P, UK 2C 167173-88-8P,
 UK 2D
 RL: PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
 (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel
 antifungal antibiotics from Streptomyces sp. 517-02)
 RN 167173-86-6 CA
 CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-
 pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-
 7-yl ester, (2E)- (9CI) (CA INDEX NAME)

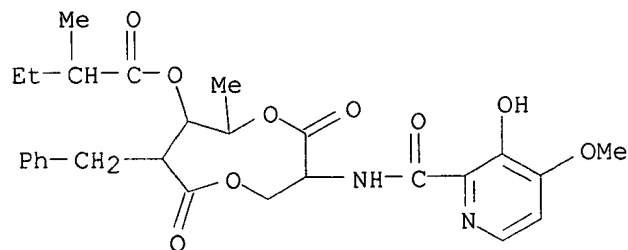
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 167173-87-7 CA
CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



RN 167173-88-8 CA
CN Butanoic acid, 2-methyl-, 3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



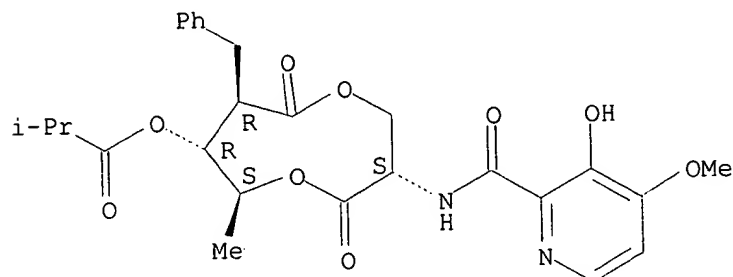
IT 167173-85-5P
RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant);
PREP (Preparation)

(structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from *Streptomyces* sp. 517-02)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



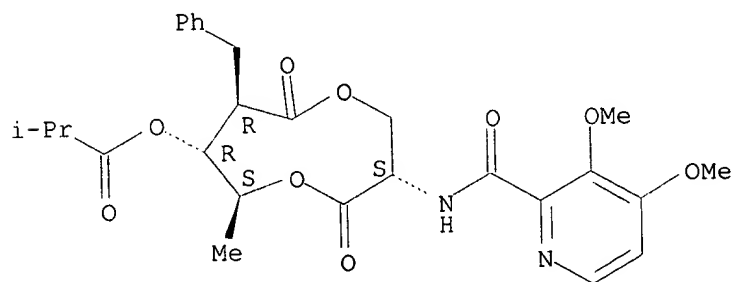
IT 186528-19-8P, O-Methyl UK 2A

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from *Streptomyces* sp. 517-02)

RN 186528-19-8 CA

CN Propanoic acid, 2-methyl-,
3-[[[(3,4-dimethoxy-2-pyridinyl)carbonyl]amino]-
6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester,
[3S-(3R*,6R*,7S*,8S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 7 OF 9 CA COPYRIGHT 2000 ACS

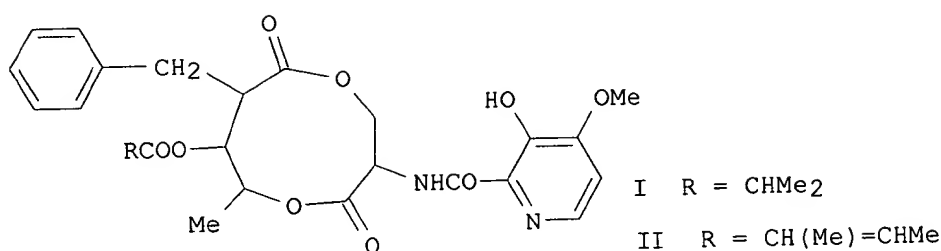
ACCESSION NUMBER: 125:109869 CA

TITLE: UK-2A, B, C and D, novel antifungal antibiotics from *Streptomyces* sp. 517-02. I. Fermentation, isolation, and biological properties

AUTHOR(S): Ueki, Masahi; Abe, Keiichi; Hanafi, Muhammad;
Shibata,

Kozo; Tanaka, Toshio; Taniguchi, Makoto
CORPORATE SOURCE: Fac. Science, Osaka City Univ., Osaka, 558, Japan

SOURCE: J. Antibiot. (1996), 49(7), 639-643
 CODEN: JANTAJ; ISSN: 0021-8820
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Novel antifungal antibiotics, UK-2A (I), UK-2B (II) and a mixt. of UK-2C and UK-2D, were obtained from the mycelial cake of *Streptomyces* sp. 517-02. All of the UK-2 compds. were similar in structure to antimycin

A. The antifungal activities of of UK-2 compds. were as strong as that of antimycin A. However, the UK-2 compds. demonstrated weak cytotoxicity compared to antimycin A.

IT 167173-85-5, UK 2A 167173-86-6, UK 2B
 167173-87-7, UK 2C 167173-88-8, UK 2D

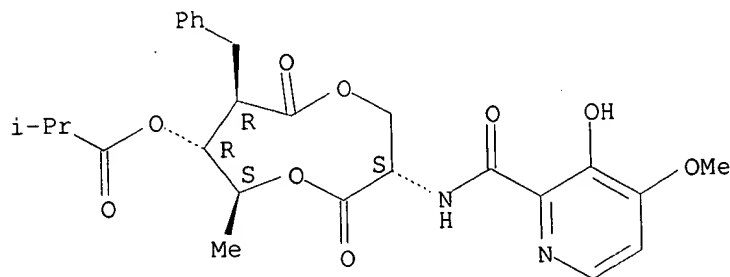
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)

(UK-2A, B, C and D, novel antifungal antibiotics from *Streptomyces* sp. 517-02. I. Ferment., isolation, and biol. properties)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

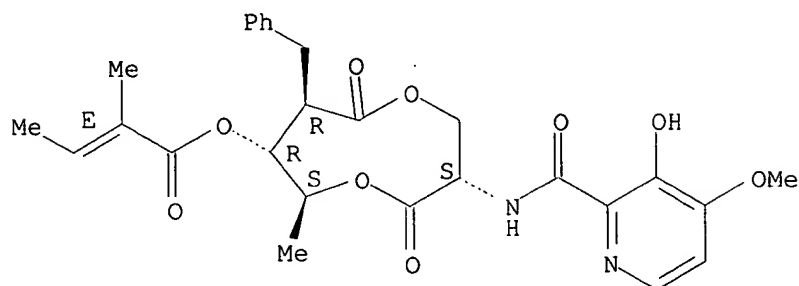


RN 167173-86-6 CA

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-

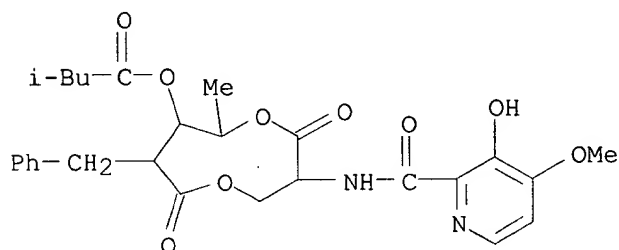
7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



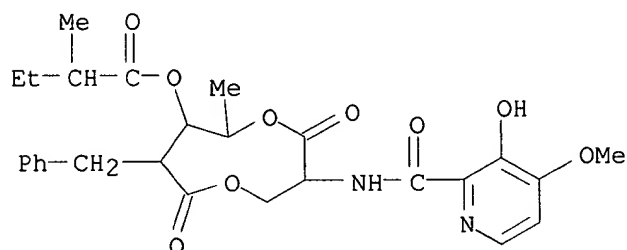
RN 167173-87-7 CA

CN Butanoic acid, 3-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8- (phenylmethyl)-1, 5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8- (phenylmethyl)-1, 5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

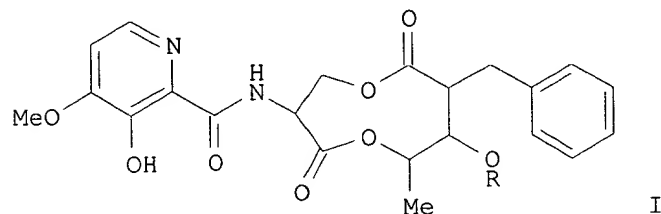


L9 ANSWER 8 OF 9 CA COPYRIGHT 2000 ACS
ACCESSION NUMBER: 123:337552 CA

TITLE: Fungicides manufacture with Streptoverticillium
 INVENTOR(S): Taniguchi, Makoto; Shibata, Kozo; Abe, Keiichi;
 Kodama, Tooru; Uotani, Kazumichi; Oonishi, Yoshitaka
 PATENT ASSIGNEE(S): Suntory Ltd, Japan; Meiji Seika Co
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07233165	A2	19950905	JP 1994-26884	19940224 <--

OTHER SOURCE(S): MARPAT 123:337552
 GI



AB Fungicides (I: R = linear or branched aliph. (un)satd. acyl group) are manufd. by culturing Streptoverticillium sp. SAM2084. Shake-culture of Streptoverticillium sp. SAM2084 for manuf. of four I wherein R = 2-methylpropanoyl (UK-2A), trans-2-methyl-2-butenoyl (UK-2B), 3-methylbutanoyl (UK-2C), and 2-methylbutanoyl (UK-2D) was shown. Also given were the physiol. and morphol. characteristics of the Streptoverticillium sp. SAM2084.

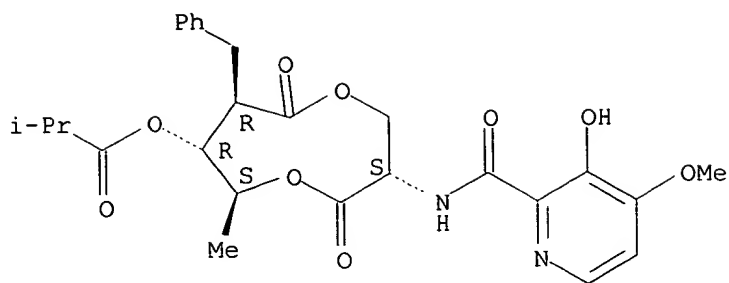
IT **167173-85-5P**, UK 2A **167173-86-6P**, UK 2B
167173-87-7P, UK 2C **167173-88-8P**, UK 2D

RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (fungicides manuf. with Streptoverticillium)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

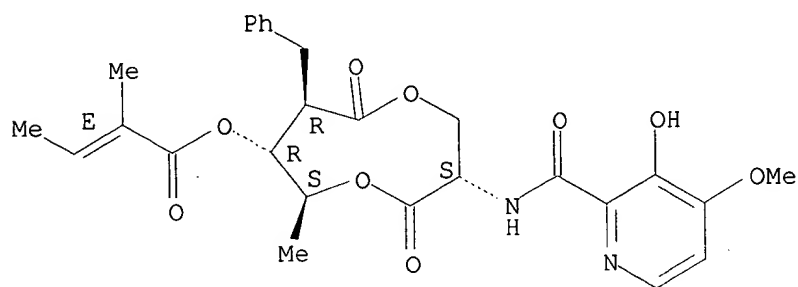
Absolute stereochemistry. Rotation (+).



RN 167173-86-6 CA

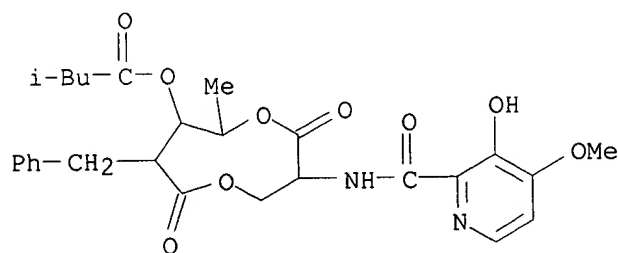
CN 2-Butenoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8- (phenylmethyl)-1, 5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



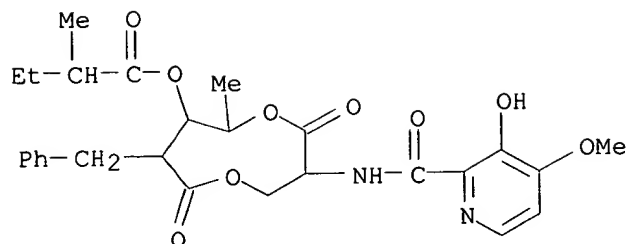
RN 167173-87-7 CA

CN Butanoic acid, 3-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8- (phenylmethyl)-1, 5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8- (phenylmethyl)-1, 5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



L9 ANSWER 9 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER: 123:164736 CA

TITLE: The structures of UK-1 and UK-2, novel antibiotics from *Streptomyces* sp. 517-02

AUTHOR(S): Hanafi, O Muhammad; Kozo, Shibata; Masaru, Kashiwada; Masashi, Ueki; Makoto, Taniguchi

CORPORATE SOURCE: Faculty Science, Osaka City University, Japan

SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (

1994), 36th, 728-35

CODEN: TYKYDS

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB The mycelial cake was extd. with acetone, and filtered. The filtrate was concd. to give aq. soln., which was extd. with chloroform. Org. layer was

concd. to yield an oily material, followed by purifn. on silica gel column

chromatog. to give crude UK-1 and UK-2. Finally, the recrystn. of each fractions from MeOH, afforded UK-1 and UK-2. UK-1 (I), a novel metabolite, demonstrated potent cytotoxic activity against B16, Hela and P388 cells, and UK-2, novel complex of antibiotics, exhibited strong antifungal activity. Methylation of UK-1 by CH3I and anhyd. K2CO3 in dry acetone gave monomethyl ether deriv., Me-UK-1. Alk. hydrolysis of UK-1 afforded carboxylic acid deriv., DeMe-UK-1. Partial structures, A, B,

and C were elucidated by COSY, and COLOC expts. Based on these results, the structure of UK-1 was deduced to be a novel benzoxazole dimer deriv.

UK-2, novel metabolite contg. complex of antibiotics with strong antifungal activity, was purified by reverse phase HPLC, to give UK-2A,

B, C and D. From NMR and mass spectral data, the structures of UK-2A, B, C and D were established as isobutyrate, tiglate, isovalerate, and 2-methylbutyrate of nine membered dilactone skeleton, resp. Based on the result of synthesis of hydrolysis products, the abs. configuration of

UK-2 was identified.

IT 167173-85-5, Antibiotic UK 2A 167173-86-6, Antibiotic UK

2B 167173-87-7, Antibiotic UK 2C 167173-88-8,

Antibiotic UK 2D

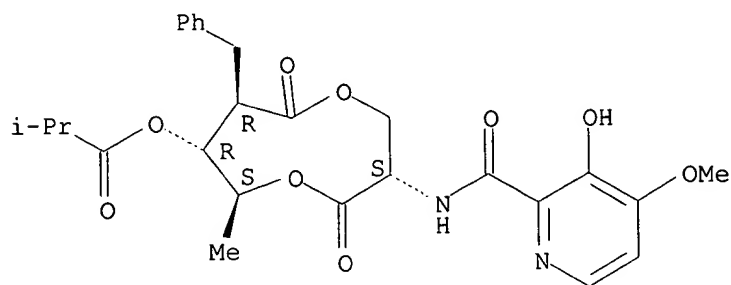
RL: PRP (Properties)

(structures of UK-1 and UK-2, novel antibiotics from *Streptomyces* sp. 517-02)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

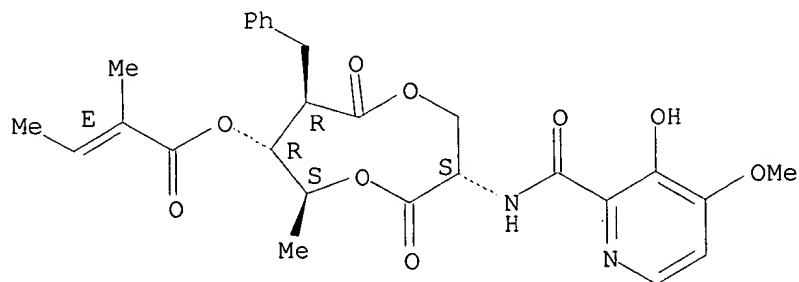
Absolute stereochemistry. Rotation (+).



RN 167173-86-6 CA

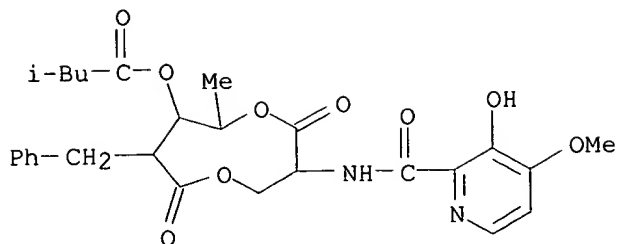
CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 167173-87-7 CA

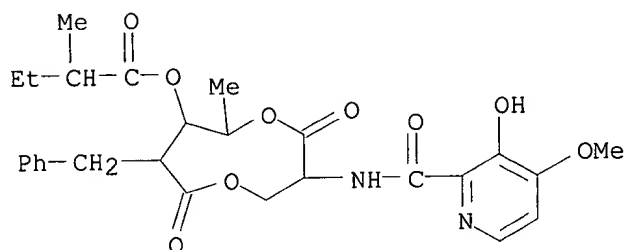
CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[[3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
49.24	176.59

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
-6.36	-6.36

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L1 STRUCTURE UPLOADED
L2 7 S L1
L3 STRUCTURE UPLOADED
L4 4 S L3
L5 75 S L4 FULL

FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000

L6 14 S L5
L7 3 S L6 AND SAKANAKA, O?/AU
L8 11 S L6 NOT L7
L9 9 S L8 AND PD < MARCH 1998

FILE 'CAOLD' ENTERED AT 12:44:17 ON 02 NOV 2000

=> s 15

L10 0 L5

=> d his

(FILE 'HOME' ENTERED AT 12:39:26 ON 02 NOV 2000)

FILE 'REGISTRY' ENTERED AT 12:39:46 ON 02 NOV 2000

L1 STRUCTURE UPLOADED
L2 7 S L1
L3 STRUCTURE UPLOADED
L4 4 S L3
L5 75 S L4 FULL

FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000

L6 14 S L5
L7 3 S L6 AND SAKANAKA, O?/AU
L8 11 S L6 NOT L7
L9 9 S L8 AND PD < MARCH 1998

FILE 'CAOLD' ENTERED AT 12:44:17 ON 02 NOV 2000

L10 0 S L5

=>

---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.30	176.89
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-6.36

STN INTERNATIONAL LOGOFF AT 12:45:01 ON 02 NOV 2000

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International! Enter x:x

LOGINID:ssspal612BXR

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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NEWS	7	Sep 21	KKF renamed DKILIT
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FULL ESTIMATED COST	0.15	0.15

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STRUCTURE FILE UPDATES: 1 NOV 2000 HIGHEST RN 300762-14-5
 DICTIONARY FILE UPDATES: 1 NOV 2000 HIGHEST RN 300762-14-5

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
 for details.

=> e tigloyl/cn

```

E1          1      TIGLOPHORBOL T/CN
E2          1      TIGLOSIDE/CN
E3          0 --> TIGLOYL/CN
E4          1      TIGLOYL CHLORIDE/CN
E5          1      TIGLOYL PSEUDOTROPINE/CN
E6          1      TIGLOYL-COA/CN
E7          1      TIGLOYL-COA-3.BETA., 13.ALPHA.-DIHYDROXYLUPANINE
13-O-TIGLOYL
              TRANSFERASE/CN
E8          1      TIGLOYL-COA-PSEUDOTROPINE ACYLTRANSFERASE/CN
E9          1      TIGLOYL-COA-TROPINE ACYLTRANSFERASE/CN
E10         1      TIGLOYL-COA: 13-HYDROXYLUPANINE O-TIGLOYLTRANSFERASE/CN
E11         1
TIGLOYL-COA: (-)-13.ALPHA.-HYDROXYMULTIFLORINE/(+)-13.ALPHA.-
              HYDROXYLUPANINE O-TIGLOYLTRANSFERASE/CN
E12         1      TIGLOYL-COA: 13.ALPHA.-HYDROXYLUPANINE
O-TIGLOYLTRANSFERASE/C
              N
  
```

=> s e4

L1 1 "TIGLOYL CHLORIDE"/CN

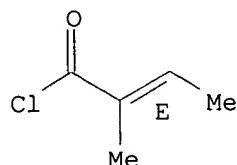
=> d l1

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L1  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2000 ACS
RN  35660-94-7  REGISTRY
CN  2-Butenoyl chloride, 2-methyl-, (2E)- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  2-Butenoyl chloride, 2-methyl-, (E)-
CN  Tigloyl chloride (6CI, 7CI)
OTHER NAMES:
CN  (E)-2-Methyl-2-butenoyl chloride
  
```

CN Tiglic acid chloride
 FS STEREOSEARCH
 MF C5 H7 Cl O
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CSCHEM, SPECINFO, TOXLIT, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)

Double bond geometry as shown.



74 REFERENCES IN FILE CA (1967 TO DATE)
 74 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e isopropyl/cn

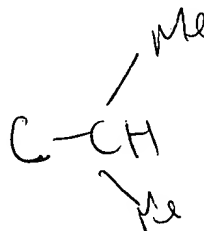
E1	1	ISOPROPYLYL (PHENYLIMINO)ACETATE/CN
E2	1	ISOPROPYDRIN/CN
E3	1 -->	ISOPROPYLYL/CN
E4	1	ISOPROPYLYL ((2-BROMOETHYL) THIO)ACETATE/CN
E5	1	ISOPROPYLYL
		((4-CHLOROPHENYL) AMINO) IMINOMETHYLCARBAMIMIDATE/CN
E6	1	ISOPROPYLYL ((4-METHOXYPHENYL) IMINO)ACETATE/CN
E7	1	ISOPROPYLYL ((CHLOROMETHYL) THIO)ACETATE/CN
E8	1	ISOPROPYLYL ((PERHYDROAZEPINO) METHYL) (METHYL) PHOSPHINATE/CN
E9	1	ISOPROPYLYL (+)-2-CHLOROPROPIONATE/CN
E10	1	ISOPROPYLYL (.+-.)-.ALPHA.-ISOCYANOPROPIONATE/CN
E11	1	ISOPROPYLYL (.+-.)-3-OXOCYCLOHEXANECARBOXYLATE/CN
E12	1	ISOPROPYLYL (.+-.)-CIS-CRYSANTHEMATE/CN

=> s e3

L2 1 ISOPROPYLYL/CN

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2000 ACS
 RN 2025-55-0 REGISTRY
 CN Ethyl, 1-methyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN **Isopropyl** (6CI, 8CI)
 OTHER NAMES:
 CN 1-Methylethyl
 CN 2-Propyl
 CN 2-Propyl radical



CN iso-Propyl
 CN iso-Propyl radical
 CN Isopropyl radical
 MF C3 H7
 LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD,
 CAPLUS,
 CASREACT, CEN, CIN, GMELIN*, PIRA, PROMT, TOXLIT, TRCTHERMO*, USPATFULL
 (*File contains numerically searchable property data)

H₃C-CH-CH₃

427 REFERENCES IN FILE CA (1967 TO DATE)
 6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 427 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 40 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e isovaleryl.cn

E1	1	ISOVALERY/BI
E2	988	ISOVALERYL/BI
E3	0 -->	ISOVALERYL.CN/BI
E4	6	ISOVALERYLACET/BI
E5	1	ISOVALERYLACETATE/BI
E6	1	ISOVALERYLACETIC/BI
E7	1	ISOVALERYLACETO/BI
E8	4	ISOVALERYLACETONE/BI
E9	1	ISOVALERYLACETOPHEN/BI
E10	1	ISOVALERYLACETOPHENONE/BI
E11	1	ISOVALERYLADENOSINE/BI
E12	1	ISOVALERYLADRENAL/BI

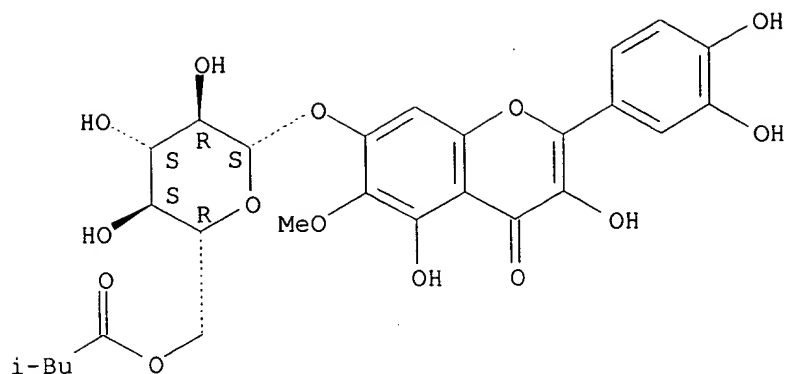
=> s e2

L3 988 ISOVALERYL/BI

=> d l3, 1

L3 ANSWER 1 OF 988 REGISTRY COPYRIGHT 2000 ACS
 RN 254879-11-3 REGISTRY
 CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-6-methoxy-7-
 [[6-O-(3-methyl-1-oxobutyl)-.beta.-D-glucopyranosyl]oxy]- (9CI) (CA
 INDEX
 NAME)
 OTHER NAMES:
 CN **Patuletin 7-O-(6''-isovaleryl)glucoside**
 FS STEREOSEARCH
 MF C27 H30 O14
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 13:00:52 ON 02 NOV 2000)

FILE 'REGISTRY' ENTERED AT 13:00:59 ON 02 NOV 2000

E TIGLOYL/CN
L1 1 S E4
E ISOPROPYL/CN
L2 1 S E3
E ISOVALERYL.CN
L3 988 S E2

=> e isovaleryl/cn

E1 1 ISOVALEROYL-COENZYME A DEHYDROGENASE/CN
E2 1 ISOVALEROYLPENTAMETHYLBENZENE/CN
E3 1 --> ISOVALERYL/CN
E4 1 ISOVALERYL ANHYDRIDE/CN
E5 1 ISOVALERYL AZIDE/CN
E6 1 ISOVALERYL CHLORIDE/CN
E7 1 ISOVALERYL COA DEHYDROGENASE/CN
E8 1 ISOVALERYL COENZYME A/CN
E9 1 ISOVALERYL DIETHYLAMIDE/CN
E10 1 ISOVALERYL FLUORIDE/CN
E11 1 ISOVALERYL ISOTHIOCYANATE/CN
E12 1 ISOVALERYL L-CARNITINE/CN

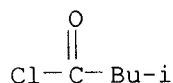
=> s e6

L4 1 "ISOVALERYL CHLORIDE"/CN

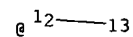
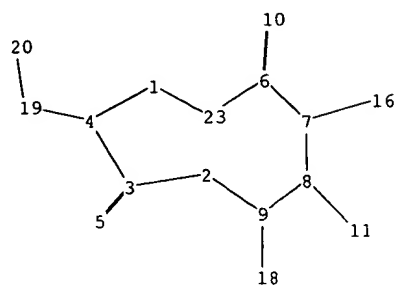
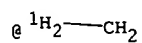
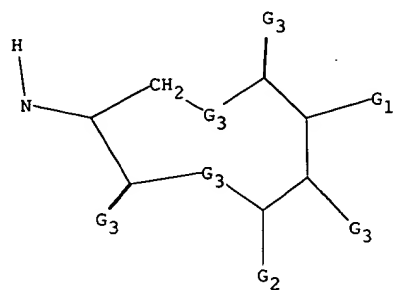
=> d 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2000 ACS
RN 108-12-3 REGISTRY

CN Butanoyl chloride, 3-methyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN **Isovaleryl chloride** (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN 3-Methylbutanoyl chloride
 CN 3-Methylbutyryl chloride
 CN Isopentanoyl chloride
 CN Isovaleric acid chloride
 CN Isovaleric chloride
 CN Isovaleroyl chloride
 FS 3D CONCORD
 MF C5 H9 Cl O
 LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, HODOC*, IFICDB, IFIPAT,
 IFIUDB,
 MRCK*, MSDS-OHS, SPECINFO, TOXLINE, TOXLIT, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



612 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 614 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)



chain nodes :

5 10 11 12 13 16 18 19 20

ring nodes :

1 2 3 4 6 7 8 9 23

chain bonds :

3-5 4-19 6-10 7-16 8-11 9-18 12-13 19-20

ring bonds :

1-4 1-23 2-3 2-9 3-4 6-7 6-23 7-8 8-9

exact/norm bonds :

1-4 1-23 2-3 2-9 3-4 3-5 4-19 6-10 6-7 6-23 7-8 7-16 8-9 8-11 9-18 12-13
19-20

isolated ring systems :

containing 1 :

G1:CH2, [*1]

G2:CH3, Et

G3:O, S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:CLASS 13:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS 23:Atom

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International! Enter x:x
 LOGINID:sssptal612BXR
 PASSWORD:
 TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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NEWS	3	Aug 24	TABULATE Now Available in More STN Databases
NEWS	4	Aug 28	MEDLINE from 1958 to Date - Only on STN
NEWS	5	Sep 7	DGENE GETSIM ALERT: Similarity Current-Awareness Searching of Biosequences
NEWS	6	Sep 11	Textile Technology Digest (TEXTILETECH) now available on STN
NEWS	7	Sep 21	KKF renamed DKILIT
NEWS	8	Sep 29	The Philippines Inventory of Chemicals and Chemical Substances (PICCS) has been added to CHEMLIST
NEWS	9	Oct 27	New Extraction Code PAX now available in Derwent Files
NEWS	10	Oct 27	SET ABBREVIATIONS and SET PLURALS extended in Derwent World Patents Index files
NEWS	11	Oct 27	Patent Assignee Code Dictionary now available in Derwent Patent Files
NEWS	12	Oct 27	Plasdoc Key Serials Dictionary and Echoing added to Derwent Subscriber Files WPIDS and WPIX
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* * * * * STN Columbus * * * * *

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.15

0.15

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STRUCTURE FILE UPDATES: 1 NOV 2000 HIGHEST RN 300762-14-5
 DICTIONARY FILE UPDATES: 1 NOV 2000 HIGHEST RN 300762-14-5

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
 for details.

=>

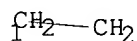
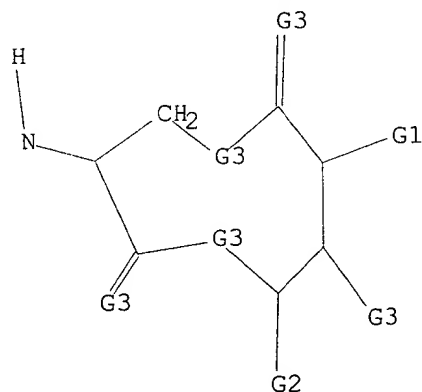
Uploading 9601655c.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 CH2, [01]

G2 Me, Et

G3 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 13:29:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5283 TO ITERATE

18.9% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 101308 TO 110012
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l2 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 126.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 13:30:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 104836 TO ITERATE

100.0% PROCESSED 104836 ITERATIONS 75 ANSWERS
SEARCH TIME: 00.00.04

L3 75 SEA SSS FUL L1

=> file ca

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	126.60	126.75

FILE 'CA' ENTERED AT 13:30:20 ON 02 NOV 2000
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FILE COVERS 1967 - 27 Oct 2000 VOL 133 ISS 19
FILE LAST UPDATED: 27 Oct 2000 (20001027/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in CA on STN.

=> s 13

L4 14 L3

=> save title

ENTER L#, L# RANGE, ALL, OR (END):14

ENTER NAME OR (END):anti655/a

ENTER TITLE (NONE):broad search 11/2/00

ANSWER SET L4 HAS BEEN SAVED AS 'ANTI655/A'